



Contribution ID: 225

Type: Poster

Ab initio Calculations of Phonon Spectra in PtCr Binary

We investigate the thermal stability at 0 GPa for different phases of PtCr binary alloys. We have detected soft modes at X, G, M and R points of the Brillouin zone from the phonon spectra of Pt₃Cr A15 phase. Pt₃Cr L12 and PtCr₃ A15 are predicted as dynamically stable structures.

Primary author: Mrs TIBANE, Malebo (University of South Africa)

Co-author: Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: Mrs TIBANE, Malebo (University of South Africa)

Track Classification: Track A - Condensed Matter Physics and Material Science